1,2-Cyclohexanedicarboxylic acid, 3-pentyl tetradecyl ester

Inchi: InChI=1S/C27H50O4/c1-4-7-8-9-10-11-12-13-14-15-16-19-22-30-26(28)24-20-17-18-21-

InchiKey: VPIULOFZSQRDKD-UHFFFAOYSA-N

Formula: C27H50O4

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)CC

Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-277.08	kJ/mol	Joback Method
hf	-1061.51	kJ/mol	Joback Method
hfus	60.64	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.769		Crippen Method
mcvol	395.310	ml/mol	McGowan Method
pc	798.89	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	984.18	K	Joback Method
tc	1206.59	K	Joback Method
tf	526.51	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.73	J/mol×K	984.18	Joback Method
cpg	1492.66	J/mol×K	1169.52	Joback Method
cpg	1480.00	J/mol×K	1132.45	Joback Method
cpg	1465.52	J/mol×K	1095.39	Joback Method
cpg	1449.19	J/mol×K	1058.32	Joback Method
cpg	1430.94	J/mol×K	1021.25	Joback Method
cpg	1503.56	J/mol×K	1206.59	Joback Method
dvisc	0.0000231	Pa×s	984.18	Joback Method

dvisc	0.0000312	Pa×s	907.90	Joback Method
dvisc	0.0000444	Pa×s	831.62	Joback Method
dvisc	0.0000680	Pa×s	755.35	Joback Method
dvisc	0.0001144	Pa×s	679.07	Joback Method
dvisc	0.0002198	Pa×s	602.79	Joback Method
dvisc	0.0005103	Pa×s	526.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339511&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume